PG Diploma in Cheminformatics Syllabus UNIVERSITY DEPARTMENT Program Code: **** 2021 – 2022 onwards

BHARATHIAR UNIVERSITY

(A State University, Accredited with "A" Grade by NAAC, Ranked 13th among Indian Universities by MHRD-NIRF, World Ranking : Times - 801-1000, Shanghai - 901-1000, URAP – 1047)

Coimbatore - 641 046, Tamil Nadu, India

Program	Educational Objectives (PEOs)
	Diploma in Cheminformatics program describe accomplishments that graduates are to attain within five to seven years after graduation
PEO1	Should be aware of available Cheminformatics resources and information in databases
PEO2	Apply critical, analytical and problem solving skills to deal with Cheminformatics research
PEO3	Gain a deep understanding of the biomolecular systems
PEO4	Attain knowledge to identify the research problems in Cheminformatics
PEO5	Develop very efficient algorithms to extract biological knowledge from complex dataset
PEO6	Develop programming skills to write their own codes and scripts to resolve research accomplishments
PEO7	Possess drafting and writing skills to enhance scientific communication
PEO8	Update in accordance with recent scientific advancements and technology
PEO9	Gain higher level degrees to pursue a career in academics or scientific organizations
PEO10	Should be able to pursue research and also in industry placement in the sectors of pharmaceutical, agricultural, environmental science and food industries

Program	Specific Outcomes (PSOs)
After the expected	successful completion of PG Diploma in Cheminformatics program, the students are to
PSO1	Develop applications to solve biological problems by utilizing the Cheminformatics algorithms and programming languages
PSO2	Manipulate scientific datasets and retrieve and access them through biological databases
PSO3	Develop knowledge and skills to analyses and interpret biological data for research requirements
PSO4	Develop good scientific communication skills
PSO5	Gain knowledge of the tools, frameworks, and libraries for Cheminformatics applications
PSO6	Undergo seminars, conferences and hands on workshops to facilitate domain expertise



Program	Outcomes (POs)
On succe	ssful completion of the M. Sc. Bioinformatics program
PO1	Should be able to understand the basic principles and concepts of biology, chemistry, computer science and mathematics
PO2	Able to apply the knowledge in Cheminformatics such as computational biology, chemical principles that underlie biochemistry, molecular biology and genomics
PO3	Develop and implement software effectively to retrieve information from biological databases and use this information for computation
PO4	Comprehend and provide solution to enable designing and implementing new algorithms and analysis methods
PO5	Understand the concept of intersection of life and information sciences, structure- function relationships, information theory, gene expression, and database queries
PO6	Develop computational techniques and diversified bioinformatics tools for processing data, including statistical, machine learning and data mining techniques
PO7	Design and implement efficient and reliable Cheminformatics solutions by optimizing the usage of existing tools and developing new ones
PO8	Analyze and think critically the research methods in Cheminformatics such as dissertation, research, preparation and presentations at scientific meetings, seminars and qualifying examinations
PO9	Develop an insight into scientific methodology and advances in Cheminformatics research
PO10	Have an understanding of current technology trends as well as future directions and recognize the need and develop the skills necessary for professional development

BHARATHIAR UNIVERSITY: COIMBATORE 641 046

PG Diploma in Cheminformatics

Curriculum (University Department)

(For the students admitted during the academic year 2021 – 22 onwards)

	Course	T'41, ef 41, e Comme	C l'4-	H	ours	Maxi	imum M	larks	
	Code	Title of the Course	Credits	Theory	Practical	CIA	ESE	Total	-
		F	TIRST SE	MESTER	14		I	T	
	13A	Basics of Cheminformatics	5	60	· · · ·	50	50	100	
	13B	Computer Programming for Cheminformatics	5	60		50	50	100	
	13C	Cheminformatics Database Design and Their Management	5	60	YA.	<mark>50</mark>	50	100	
	13D	Pharmaceutical Chemistry	5	60		50	50	100	
М	20	Total	20			200	200	400	
		SE	COND SI	EMESTE	R	1		m	
	23A	Structure Based Drug Design	5	60		50	50	100	17
4	23P	Practical-I: Computer Programming	5	173	60	50	50	100	, r
	23Q	Practical – II: Computer Aided Drug Design	5	- 38	60	50	50	100	
	27V	Project & Viva-Voce	10	1.1.16	Withour .	50	50	100	
		Total	25		1 Suman	200	200	400	_
		Grand Total	45	1000		400	400	800	



code	13A	<u> </u>		L	Т	Р	C
Core/Ele	ective/Suppo	rtive	Core	5	-	-	5
Pre-r	equisite		Basic Knowledge in Chemistry	Sylla Vers		202	1-22
Course Ob	ojectives:						
The main of	objectives of	this co	ourse are to:				
 Retrie To ma 	eve chemical ake students	inforr famili	secondary structures of proteins with stered nation from structural and visualization too ar on existing databases and their applicatio porithms which is involved in biomolecular	ls. on.	-		
Expected (Course Outo	comes		See.			
_			n of the course, student will be able to:	- 3			
1	Understand	l the m	nathematical implementation in molecular ne	etworks	5.		K1
2	Evaluate th	e imp	ortance of protein structure in drug designin	ng.			K2
3			al data retrieval from the databases.		÷		K3
4	14		s tools in proteomics, genomics and metabo	l <mark>om</mark> ics	. 3	S	K4
5			lesigning of ligand with a help of QSAR.				K5
Unit:1 Graph theor matrices; M	ry and molec fathematical	cular reaso	Molecular Numerology numerology; Logic, sets and functions; Al ning, induction and recursion; Counting;	lg <mark>or</mark> ith graphs	1 ms, in s, tree	2 hounteger	rs s and sets
Unit:1 Graph theor matrices; M	ry and molec lathematical ability and	cular reaso	Molecular Numerology numerology; Logic, sets and functions; Al	lg <mark>or</mark> ith graphs	1 ms, in s, tree	2 hounteger	rs s and sets
Unit:1 Graph theor matrices; M basic proba Metabolic P Unit:2	ry and molect lathematical ability and Pathways.	cular reaso statis	Molecular Numerology numerology; Logic, sets and functions; Al ning, induction and recursion; Counting; tics; Markov processes. Application: B Stereochemistry	lgorith graphs iomole	1 ms, in s, tree ecule 1	2 hou nteger s and Netv 2 hou	rs s and sets vorks rs
Unit:1 Graph theor matrices; M basic proba Metabolic P Unit:2 Basic Stered acids and b Tertiary str structures. In Unit:3 History of chemical in searching-ar	ry and molect lathematical ability and Pathways. ochemistry, pases; Protein ructure; Qua ntroduction t scientific in nformation nalytical che	cular reaso statis statis Amin n stru aternar to drug nform searcl emistr	Molecular Numerology numerology; Logic, sets and functions; Al ning, induction and recursion; Counting; tics; Markov processes. Application: B	lgorith graphs iomole iomole , pH a cture force	1 ms, in s, tree ecule 1 nd io - heli s tha 1 cal in ne an ndustr	2 hou nteger s and Netv 2 hou onizati x & t ma 2 hou nform d fo ry so	rs s and sets vorks rs on o sheet intain rs ation
Unit:1 Graph theor matrices; M basic proba Metabolic P Unit:2 Basic Stered acids and b Tertiary str structures. In Unit:3 History of chemical in searching-ar Chemical St	ry and molect lathematical ability and Pathways. ochemistry, pases; Protein ructure; Qua ntroduction t scientific in nformation nalytical che	cular reaso statis statis Amin n stru aternar to drug nform searcl emistr	Molecular Numerology numerology; Logic, sets and functions; Al ning, induction and recursion; Counting; tics; Markov processes. Application: B Stereochemistry o acids and Proteins and Properties; pKa acture - Primary structure, Secondary stru- ry structure; covalent and non-covalent g action, pro drug design and applications. Chemical Information ation communication-chemical literature- h-chemical information sources-chemical ry-chemical history-biography-directories s, Formats, Drawing Tools and Structure Vis	lgorith graphs iomole iomole , pH a cture force	1 ms, in s, tree ecule 1 nd io - heli s tha 1 cal in the an ndustri ttions.	2 hou nteger s and Netv 2 hou onizati x & it ma 2 hou nform id fo ry so	rs on o sheet intain rmula urces
Unit:1 Graph theor matrices; M basic proba Metabolic P Unit:2 Basic Stered acids and b Tertiary str structures. In Unit:3 History of chemical in searching-ar Chemical St Unit:4 Introduction available d Proteomics;	ry and molec lathematical ability and Pathways. ochemistry, oases; Protein ructure; Quantroduction t scientific in nformation nalytical che tructure: Data n to data and atabases; D Metabolom Pymol or CH	cular reaso statis Amin n stru aternar to drug nform searcl emistr abases Datab vatabas sics; V	Molecular Numerology numerology; Logic, sets and functions; Al ning, induction and recursion; Counting; tics; Markov processes. Application: B Stereochemistry o acids and Proteins and Properties; pKa acture - Primary structure, Secondary stru- ry structure; covalent and non-covalent g action, pro drug design and applications. Chemical Information ation communication-chemical literature- h-chemical information sources-chemical ry-chemical history-biography-directories	lgorith graphs iomole , pH a cture force -chemid and in sualiza	1: ms, in s, tree ecule 1: und io - heli s tha 1: cal in tions. 1 cal dat Gen struc	2 hou nteger s and Netv 2 hou onizati x & t ma 2 hou nform d fo ry so 2 hou cy so 2 hou	rs s and s sets vorks rs on o sheet intain rs ation rmula urces urs blicly s and using

structure, Drug action & enzymes. Drug action & receptors, Drug Design, Ligand-Based Design and De Novo Drug Design Virtual screening/docking of ligands. Pharmacophore Design, Molecular similarity and molecular descriptors. Prediction of Binding Modes, Protein-Ligand binding free energies, ADMET prediction, QSAR and 3D-QSAR Methods.

						Tota	al Lectur	re hours	6	0 hours
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Refere			Matha	la fan Di		" A uflease	Acadam	Duese 100) <i>5</i>	
1	Maine	ematical	Method	is for Pl	nysicists	Ariken,	Academ	ic Press 198	55	
		m's Outli inivasan		Probabil	ity and	Statistics,	Murray	R Spiegel,	John J. S	Schiller, F
3	Stereo	chemistr	y, by D	avid G.	Morris,	Eddie Ab	oel	States		
		69.			-	-		Branden, Jo	2	
	James	F. Kerwi	in	500	1			ug Discove	3	
6	Compi	iter-Aide	d Drug	Design	: Metho	ds and Aj	pplication	ns, T.J. Peru	n C.L. Pr	ropst
	Chemi Wiggii		rmation	Source	es (Mcg	raw-Hill	Series i	n Advanced	1 Chemis	stry) ,Gai
8	Introdu	action to	Bioinfo	ormatics	s, Teresa	K. Attwo	ood, Dav	id Parry-Sm	iith	
			0		-	les and n, Gerd F		ions, 3rd	Edition,H	lans-Diete
	Trends India.	in Bioi	nforma	tics. By	Dr. P.	Shanmug	ghavel. 2	006 Pointer	publishe	ers, Jaipu
	Princ <mark>ir</mark> India.	bles of B	ioinfor	natics.	<mark>By</mark> Dr. P	. Shanmu	ighavel.	2005 Pointe	r publish	ers, Jaipu
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Course	Design	ned By:	Dr.P.Sh	anmugl	havel &	Dr. <mark>V.He</mark> r	namalini		14	£ 3
Mappin	ng with	n <mark>Progra</mark>	mme O	outcom	es		-	- 23		51.9
COs	PO1	PO2	PO3	PO4	PO5	PO6	PO7	PO8	PO9	PO 10
C01	S	S	S	S	М	S	М	S	S	М
CO3	М	М	М	S	S	M	S	М	М	Μ
CO3	S	М	S	S	М	S	М	S	S	S
CO4				S						

*S-Strong; M-Medium; L-Low

CO5

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Course	13B	COMPUTER PROGRAMMING FOR	L	Т	Р	С
code		CHEMINFORMATICS	Ľ	1	1	C
Core/Elec rtive	tive/Suppo	Core	5	-	-	5
_		Basic Knowledge in Programming	Syllabı	IS	2021	L-
Pre-requ	isite		Versio	n	22	
Course O	•					
 To ur Famil 	derstand the liarize the st	E this course are to: Languages and programmes in operating system. udents in programming languages and their ap nts update in various up comings like machine lear	_	18.		
Expected	Course Out	comes:	24.			
On the su	ccessful con	npletion of the course, student will be able to:	- 3.			
1 Unc	lerstand vari	ous terminologies in computer languages.	- 37		K	[1
2 Hav	re a good und	derstanding in the concepts of C & C++.	1		K	2
3 Obj	ective orient	ed JAVA programming in cheminformatics.			K	2
4 Be a	able to perfor	rm programming in PERL & PYTHON.		3.8	K	6
5 Crea	ate awarenes	s and familiar on Machine Learning.		-	K	6
K1 - Ren	nember; K2	- Understand; K3 - Apply; K4 - Analyze; <mark>K5 -</mark> Eva	uluate; K	<mark>6 - C</mark> re	eate	
and error-l	nandling, So	FML, XML: Key terminology, Characters and escchemas and validation Related specifications,chemical Markup Language.	-			
	1		14	- 4	2	323
Unit:2		Basics of C & C++	T	_	hou	_
Basic Expr and Scope - Casts – Pre	essions - Flo - Arrays - C	Basic Syntax - Variables, Constants and Built-in ow Control and Statement Blocks - Functions and haracter Strings – Pointers - Defining New Types he Programming Process - Writing Source Code.	d Argum	ents - s and	Moc Obje	lule cts -
Unit:3		JAVA Programming			hou	
Variables, Statement H	Constants an Blocks - Fun	Introduction to Java - JavaScript for Cheminfor ad Built-in Types - Operators and Basic Expression ctions and Arguments - Modules and Scope – Arra a Types - Classes and Objects – Casts – Preprocess	ons - Flo 1ys - Cha	w Co	ntrol	an
Unit:4		Programming in PERL and PYTHON		12	hou	rs
	ng in PERI	L and PYTHON: PERL: Introduction, Basic	operator			
structures, s Subroutines flow-modul	Scalars, List s, Text and s les-basic I/C	s, Hashes, File Manipulation, Pattern Matching ar string Processing Python Programming: Overview D, Exception Handling, Regular expressions, File	nd Regula -Data str	ar Exp ucture	oress es-co	ions ntro
standard lib	rary.	Page 8 of 18				

Unit	::5		Ι	Machine	Learnin	g				12 hours
Machi	ne Learnin	g: Defi	nition o	f learnin	g. Repres	entation	and prid	or knowl	edge. Nei	aral Networks
Superv	vised, Unsu	apervise	ed, and s	Semi-Su	pervised	Learning	g, Deep l	Learning	and Line	ar Regressior
Algori	thms and	Model	Selection	on: Line	ar Regre	ession, L	inear R	egressior	n Assessr	nent, Logisti
Regres	sion, Naiv	e Baye	s; Evalu	ating and	d choosin	g the be	st hypotl	nesis; Mo	odel selec	tion.
						Total	Lecture	hours		60 hours
Refe	erence Boo									
1	Introducti	ion to N	Aachine	Learning	g. E.Alpa	ydin, 3 rd	Edition	, 2014, N	IIT Press	
2	The Mach	nine Le	arning A	Approach	– P.Balc	l <mark>i, S.</mark> Bru	nak, F.B	atch - 20	14, MIT	Press.
3	Program	ming P	erl - To	m Christ	iansen, L	arry. Wa	all Oriell	<mark>y Publi</mark> ca	ations	
4	The C Pro	ogramn	ning Lar	nguage, H	B.W.Kerr	nighan ar	nd D.M.	Ritchie 2	2nd Editic	on. Prientice
	Hall of In	dia	5	-		100			34	
5	Programm	×	ul Lou	wy Woll	Tom Chr	istionson	e Iohn	Omront	2.1 2000	0'
3	-	ning Pe	n – Lan	ry wall,	Tom Chi	istiansei		Orwant	3ed 2000	- 0
	Reilly.	×	11	· •	1263	e. "		1		
6	Programm	ning Py	vthon - I	Mark Lut	tz – 2nd I	Ed., O' F	Reilly			
7	E. Balagu	i <mark>rusa</mark> my	/ - "Prog	grammin	g in C++	" - Tata	Mc. Gra	w Hill E	dition	1
8	B <mark>yron</mark> Go	o <mark>ttfri</mark> ed,	- "Prog	ramming	<mark>g wit</mark> h C"	(Schaur	n's Outli	ne Series	s) - Tata	
9	McGrawI	Hill Put	olishing	Compan	<mark>y - 1998</mark> .	1	570	1.203	1.2.4	
10	Object o	riented	program	nming w	ith $c++-$	Robert L	affore -	Waite ser	ries.	
		-							- 9	
Соц	rse Desigi	ned By:	Dr.N.J	evakuma	r & Dr.P	Shanmi	ighavel	10	11	
	ping with						Bilarol	/	100	203
COs	PO1	PO2	PO3	PO4	PO5	PO6	PO7	PO8	PO9	PO10
CO1	М	S	S	S	М	S	M	S	M	М
CO2	S	Μ	S	М	S	М	S	М	S	М
CO3	М	S	M	S	М	S	М	S	S	S
CO4	S	S	S	М	S	М	S	М	М	S
CO5	S	М	М	M	М	S	S	М	S	М

*S-Strong; M-Medium; L-Low

9

Course code	13C		IEMINFORMATICS DATABASE SIGN AND THEIR MANAGEMENT	L	Т	Р	C
	ective/Suppo		Core	5	_	-	5
	requisite		c Programming and Database Knowledge	Syllat Versi			21- 22
Course C	bjectives:						
	-	f this c	course are to:				
			tabases and their basic concepts.				
2. To n	nake the stud	ents ca	pable using data mining methods.				
			lity of chemical databases.				
		. R.	aller and the second				
	l Course Ou			S.			
		-	on of the course, student will be able to:				
1			rstanding of databases and its recovery.				<u>52</u>
2 3			and hierarchial data models.				<u>52</u> 51
4			tures of chemical databases.	-			K1 K4
5			methods in human genome.		1		K3
K1 - Re		_	erstand; K3 - Apply; K4 - Analyze; K5 - Ev	aluate: K	<mark>6 - C</mark>		
			, <u></u> ,			-	
Unit:1		199	Database Concepts		12	<mark>2 h</mark> ou	rs
Model and Reducing	l Normalizat E-R Diagrai	ion - 1 ms to	Il Databases-Object Databases-Basic SQL- Entity and entity sets; Relations and relations tables; Security, Backup and Recovery: (e- Recovery	onship se	ets; E	-R d	iagran
Model and Reducing raffic- Ba	l Normalizat	ion - 1 ms to	Entity and entity sets; Relations and relations tables; Security, Backup and Recovery: (e- Recovery	onship se	ets; E users	-R d - En	iagrar crypti
Model and Reducing raffic- Bad Unit:2	l Normalizat E-R Diagran ckup of the d	ion - 1 ms to atabas	Entity and entity sets; Relations and relations tables; Security, Backup and Recovery: (e- Recovery Network Data Model	onship se Creating	ets; E users	-R d - En	iagrar crypti
Model and Reducing raffic- Bac Unit:2 Network I Databases o Distribu	l Normalizat E-R Diagran ckup of the d Data Model: - Basic Con	ion - 1 ms to latabas Basic cepts a se Pro	Entity and entity sets; Relations and relations tables; Security, Backup and Recovery: (e- Recovery	onship se Creating asic Con ext Datal	ets; E users 12 cepts pases;	-R d - En 2 hou ; Mu ; Intro	iagran crypti rs ltime
Model and Reducing raffic- Bac Unit:2 Network I Databases o Distribu	l Normalizat E-R Diagran ckup of the d Data Model: - Basic Con uted Databas	ion - 1 ms to latabas Basic cepts a se Pro	Entity and entity sets; Relations and relations tables; Security, Backup and Recovery: (e- Recovery Network Data Model c concepts; Hierarchical Data Model: Ba and Applications; Indexing and Hashing; Te	onship se Creating asic Con ext Datal	ets; E users 12 cepts: bases; h dat	-R d - En 2 hou ; Mu ; Intro	iagran crypti rs ltimec oducti es; Da
Model and Reducing raffic- Bad Unit:2 Network I Databases o Distribu nteroperal Unit:3 Database	I Normalizat E-R Diagran ckup of the d Data Model: - Basic Con uted Databas pility using X	ion - 1 ms to latabas Basic cepts a se Pro KML.	Entity and entity sets; Relations and relations tables; Security, Backup and Recovery: (e- Recovery Network Data Model c concepts; Hierarchical Data Model: Ba and Applications; Indexing and Hashing; Te cessing, Data Security. Interfacing progr Database Design on to Schema Refinement- Functional Dep	onship se Creating sic Con ext Datal ams wit	ets; E users 12 cepts: bases; h dat 12 es-No	-R d - En 2 hou ; Mu ; Intro abase 2 hou prmal	iagran crypti rs ltimec oducti es; Da rs Forn
Model and Reducing raffic- Bad Unit:2 Network I Databases o Distribu nteroperal Unit:3 Database	I Normalizat E-R Diagran ckup of the d Data Model: - Basic Con uted Databas pility using X	ion - 1 ms to latabas Basic cepts a se Pro KML.	Entity and entity sets; Relations and relations tables; Security, Backup and Recovery: (e- Recovery Network Data Model c concepts; Hierarchical Data Model: Ba and Applications; Indexing and Hashing; To cessing, Data Security. Interfacing progr Database Design	onship se Creating sic Con ext Datal ams wit	ets; E users 12 cepts: bases; h dat 12 es-No	-R d - En 2 hou ; Mu ; Intro abase 2 hou prmal	iagrar crypti rs ltime oducti es; D <u>rs</u> Form
Model and Reducing raffic- Bad Unit:2 Network I Databases o Distribu nteroperat Unit:3 Database I First, Seco	I Normalizat E-R Diagran ckup of the d Data Model: - Basic Con uted Databas pility using X	ion - 1 ms to latabas Basic cepts a se Pro KML.	Entity and entity sets; Relations and relations tables; Security, Backup and Recovery: (e- Recovery Network Data Model c concepts; Hierarchical Data Model: Ba and Applications; Indexing and Hashing; Te cessing, Data Security. Interfacing progr Database Design on to Schema Refinement- Functional Dep ode, Fourth and Fifth Normal forms- Multiv	onship se Creating sic Con ext Datal ams wit	ets; E users 12 cepts bases; h dat 12 es-No	-R d -R f E hou C hou C hou C hou Dormal encie	iagran crypti rs ltimed oducti es; Da rs Forn s.
Model and Reducing raffic- Bac Unit:2 Network I Databases o Distribu nteroperal Unit:3 Database I First, Seco	I Normalizat E-R Diagran ckup of the d Data Model: - Basic Con uted Databas pility using X Design: Intro nd, Third, Bo	ion - 1 ms to latabas Basic cepts a se Pro XML.	Entity and entity sets; Relations and relations tables; Security, Backup and Recovery: (e- Recovery Network Data Model c concepts; Hierarchical Data Model: Ba and Applications; Indexing and Hashing; Te cessing, Data Security. Interfacing progr Database Design on to Schema Refinement- Functional Dep ode, Fourth and Fifth Normal forms- Multiv Chemical Databases	onship se Creating usic Con ext Datal ams wit	ets; E users 12 cepts: bases; h dat 12 es-No pende	-R d -R d -R en 2 hou 3 Intro- abase 2 hou 2 hou 2 hou	iagran crypti rs Itime oducti es; D rs Form s.
Model and Reducing raffic- Bad Unit:2 Network I Databases o Distribu nteroperat Unit:3 Database I First, Seco Unit:4 ntroductio	I Normalizat E-R Diagran ckup of the d Data Model: - Basic Con uted Databas pility using X Design: Intro nd, Third, Bo	ion - 1 ms to latabas Basic cepts a se Pro XML.	Entity and entity sets; Relations and relations tables; Security, Backup and Recovery: (e- Recovery Network Data Model c concepts; Hierarchical Data Model: Ba and Applications; Indexing and Hashing; Te cessing, Data Security. Interfacing progr Database Design on to Schema Refinement- Functional Dep ode, Fourth and Fifth Normal forms- Multiv Chemical Databases ases - types- chemical database design - B	onship se Creating asic Con ext Datal ams wit pendenci alued De io Cataly	ets; E users 12 cepts bases; h dat 12 es-No pendo 12 ysis I	-R d -R d -R En 2 hou 3 Intro 	iagrar crypti rs ltime oducti es; D rs Form s. rs ase. T
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Thematic Libraries. Biological Libraries, Bio planning, Peptide Display Libraries design and construction. **Total Lecture hours** 60 hours **Text Book(s)** Practicals in Bioinformatics By Dr. P. Shanmughavel and Gulshan Wadhwa, 2010 Pointer 1 publishers, Jaipur, India. Database Systems Concepts, Abraham Silberschatz, Henry F. Korth, S. Sudarshan 2 3 Database Management Systems, Raghu Ramakrishnan, Johannes Gehrke Data Mining Techniques, Michael Berry & Gordon Linoff 4 Course Designed By: Dr.S.Usha & Dr.C.Jayaprakash Mapping with Programme Outcomes **PO1** COs **PO2** PO₃ **PO4 PO5 PO6 PO7 PO8 PO9 PO10 CO1** S S S S S S S Μ Μ Μ **CO3** S Μ S Μ S Μ S Μ S S CO3 Μ S S S S Μ S М Μ S S S S S S S **CO4** Μ Μ S Μ S S S М Μ S S Μ **CO5** Μ Μ

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Core/Elective/	Course code 13D PHARMACEUTICAL CHEMISTRY L ore/Elective/Supportive Core 5 Pre-requisite Basic Chemistry and Knowledge in Pharma Syllabus Version ourse Objectives:	<u> </u>	-			
Pre-rea	uisite		•		2021 22	
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*		course are to:				
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Expected Cou	rse Outcome	es:				
On the succes	sful completi	ion of the course, student will be able to:	S			
1 Understar	nd the patent	and patent databases.	3.		K	2
2 To apply	biological ar	nd structural data in designing.	- 37		K	3
3 Describe	s <mark>imilarity me</mark>	ethods and clustering analysis.	1		K	3
4 Know the	e 3 <mark>D Databa</mark> s	es in Experimental and Theoretical way.			K	(4
5 conduct e	experiments (Chemical Reactions, Reaction Prediction and Synt	thesis De	sign	K	5
K1 - Rememb	er; <mark>K2</mark> - Unc	l <mark>er</mark> stand; K3 - Apply; K4 - Analyze; <mark>K5</mark> - Evaluat	e; K6 - C	Create		
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Multiobjective Library Design, Practical Examples of Library Design, High throughput screening (HTS). Chemical Reactions, Reaction Prediction and Synthesis Design.

						Tota	l Lecture	e hours		60 hours
Refer	ence Bool	ks								
1 An	Introduct	tion to C	Chemoinf	ormatics	by An	drew R.	Leach a	and Vale	erie J. Gi	llet. Spring
Pub	lisher									
2 App	lied Chei	noinform	natics - A	Achieven	nents and	d Future	Opportu	nities. Ec	lited by T	Thomas Eng
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and	Johann G	asteiger.	Wiley-V	CH publ	isher.	122				
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Cours	e Designo	ed By: D	r.S.Usha	175	1. *		194.2	Ste.		
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	lective/Suppo	ortive	Core	5	_		5
	equisite		asic Knowledge in Bioinformatics	Syllab Versio		202	1-22
Course	Objectives:			, 01,514			
The ma	in objectives of	of this c	course are to:				
1. Pr	ovide the deta	iled not	e on the strategies of Drug discovery an	d drug ac	tivity.		
2. To	describe how	to use	algorithms, to rectify our quarries.				
3. Im	plementation	of vario	ous approaches in ligand designing.				
	10 0			-			
-	ed Course Ou			C.S.			
		-	on of the course, student will be able to:		-	L	72
			gies for the activity and discovery of dru	igs.	2		<u>K3</u>
			epts of molecular dynamics.	vaia	39		K2
			proach of QSAR in Molecular field anal	ysis.	3		K3
			design approach in ligand prediction.	Last '	1. 1		K4
	Evaluate Deep docking.	p learni	ng, feature and similarity based approac	nes in mo	iecula	r K	K5
		2 - Unde	erstand; K3 - Apply; K4 - Analyze; K5	- Evaluate	: K6	- Crea	ate
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Unit:	1	11/	Drug Discovery	240	12	hou	rs
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drug dis	covery-molec	<mark>ular mi</mark>	metic- first and second generation ratio				-
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drug dis design-a Unit:2 Introduc Constan Applicat Unit:2 Develop 3D QSA receptor Unit:2 3D phan problem	covery-molect ssessment of c 2 tion, Molecul t temperature ions to protein 3 ing and using R-Introductio mapping-strue 4 macophore, I -some current	ular mi drug act ar Dyn and o n foldin QSAR n-Pharr ctural al De nov methoo	metic- first and second generation ratiivity. Molecular Dynamics amics using simple models. Dynamics constant dynamics. Conformation se g. QSAR Approach - QSAR-validation methods-3D QSAR nacophore identification-binding site m lignment and superposition-molecular fi De Novo Drug Design o Ligand design-introduction-approacl ds for de novo design.3D data base sea	approach odeling of eld analys nes to de urching an	12 ntinuc Syste QSA f unkn sis (M 12 nove	Ratic bus p matic hou R des own FA).	rs otentials search rs scriptors receptor rs g desig creening
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Feature	based a	pproa	ch, Dee	ep Learn	ing Appr	oach.				
						Total	Lecture	hours		60 hours
Refer	ence B	ooks								
1	The or	ganic o	chemis	try of dr	ug desigr	n and dru	g action,	Richard	B. Silver	rman
2	Drug d	lesign:	cutting	g edge aj	pproache	s, Darren	R. Flow	er		
3	Molec	ular M	odeling	g: Basic	Principle	s and Ap	plication	s, 3rd Ed	lition, Ha	nns-Dieter Höltje,
	Wolfg	ang Sij	opl, Di	dier Rog	gnan, Ger	d Folkers	5			
4	Molec	ular M	odellin	g: Princ	ipl <mark>es and</mark>	Applicat	<mark>tions</mark> , An	drew R.	Leach	
5	Trends	in Bio	oinform	natics. B	y Dr. P. S	Shanmug	havel. 20	006 Point	er publis	hers, Jaipur, India.
6	Princip	oles of	Bioinf	ormatics	. By Dr.	P. Shann	nughavel	. 2005 Po	ointer pul	olishers, Jaipur,
	India.									
7	Deep I	Learnir	ng for t	<mark>he</mark> Life S	Sciences:	Applyin	g Deep I	.earning	to Genor	nics, Drug
	Discov	very –	Bharatl	n Ramsu	ndar,201	9 – O'Re	eilly Publ	lishers		
		10	- /	9	100	16		1.1		2.6
		0			nughavel	& Dr.S.	Usha			
			_	e Outco		~	A			
COs	PO1	PO2	PO3	PO4	PO5	PO6	PO7	PO8	PO9	PO10
CO1	M	S	М	S	S	S	S	S	М	M
CO3	S	М	М	М	S	М	S	М	S	S
CO3	М	М	S	S	S	S	М	S	S	М
CO4	S	S	S	S	M	S	S	М	M	S
CO5	S	M	М	S	М	S	М	М	S	M

Cour	rse cod	e	23P	1			COMPU /MING		L	Т	Р	С
Core	/Elect	ive/S	Supportiv	e		Cor	e		-	-	5	5
Pre-requisite				Ba	Basic Knowledge in Programming			Syllabus Version		2021-22		
	rse Ob											
		•	ives of thi									
			erstand the	-			-	-				
			w the appl		-		-					
	3. To	mak	e students	unders	tand vari	ous codi	ng langu	ages and	their inter	nsity.		
Fyng	octod (1011P	se Outcor	noc		-						
					the cour	se, stude	nt will b	e able to:	700			
1	On the successful completion of the course, student will be able to:1To make remember the features of programs.K1											
2	-	Understand the object-oriented programming language.K1										
3			about tex	-		-		-	of tasks.	7	K	3
4			support o					*			K	6
	mo	d <mark>ul</mark> ar	rity and co	de resu	se.	2.6						
K1 -	- Reme	embe	er; K2 - U	nderstar	nd; K3 -	Apply; I	X4 - Ana	lyze; K5	- Evaluat	e; K6 -	- Cre	ate
	-	-	-	-		~			10.			
1.	C+ +						-	ogrammin	g		Ĵ.	
2.	JAV		- Class	, Object	ts and In	heritance	e	ogrammin	g			
2. 3.	JAV Perl	A	- Class - Loop	, Object , Subro	ts and In utine and	heritance I File Ha	e Indling	ogrammin	g		ļ	
2. 3. 4.	JAV Perl Pyth	A on	 Class Loop Loop 	, Object , Subro , Functi	<mark>ts and In</mark> utine and ions, Cla	heritance I File Ha sses and	e ndling Objects		0	Dialog	Dovo	
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2. 3. 4. 5.	JAV Perl Pyth Visu	A on al Ba	- Class - Loop - Loop asic - Clas - SQL op	, Object , Subro , Functi sses & (erations	ts and In utine and ions, Cla Objects, I	heritance I File Ha sses and Basic Co se Conne	e ndling Objects ontrols, F	ile Handl	ing and I	orts	Boxe	8m
2. 3. 4. 5. 6.	JAV Perl Pyth Visu MyS	A on al Ba QL	- Class - Loop - Loop asic - Clas - SQL op	, Object , Subro , Functi sses & C erations	ts and In utine and ions, Cla Objects, I , Databa	heritance I File Ha sses and Basic Co se Conno ours	e ndling Objects ntrols, F ectivity a	ile Handl	ing and I	orts		8m
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Course code	23Q	PRACTICAL – II: COMPUTER AIDED DRUG DESIGN	L	T	Р	С		
Core/Elective/	Supportive	Core	-	-	5	5		
Pre-requisite		Basic Knowledge in Bioinformatics	Syllab Versio		2021-22			
Course Object	ives:		·					
The main objec								
		types of databases and their utility to sol	ve various	quarr	ies.			
		ew chemical structures.						
3. To underst of molecul		lerive, rep <mark>resent and manipul</mark> ate the struc	tures and i	reaction	ons			
		110	1910					
Expected Cou			1000					
	-	on of the course, student will be able to:		3				
		ional modeling methods to reveal the relation properties of chemical compounds.	ationships		K	2		
	derstand the ous, liquid an	spatial structures of molecules in differe	nt states li	ke	K	2		
-	To evaluate how two or more molecular structures fit togetherK5							
	Analyzing the physical movements of atoms and molecules. K6							
K1 - Rememb	er; <mark>K2</mark> - Und	erstand; K3 - Apply; K4 - Analyze; K5 -	- Evaluate;	K6 –	Crea	te		
1 3	10.	a stranger and	10					
1 Chemie	cal database	s – ChemBank - ChemBioFinder – CSCh	nemoffice -	- ZIN	C			
2 Small N	Molecule Bu	ilding – Chemsketch, ISIS Draw	1	14				
3 Molecu	l <mark>ar Mode</mark> lin	g – Modeller, Swisspdb	1	1				
4 Molecu	llar dynamic	s - GROMACS- NAMD-VEGA ZZ		13.		23		
5 Structu	ır <mark>al ch</mark> emist	ry - NWChem –GAMESS		14	5	8		
6 Dockin	g - Auto doc	k, D <mark>OCK -VEGA-</mark> FlexX	1		18			
7 ADME	Prediction -	- SwissADME, PreADMET	1. C.	Å	÷.,	1		
8 Toxicit	y Prediction	- Toxinpred <mark>, ProTox -II</mark>			31			
9 QSAR	Prediction		Gev.	1	1			
	19	Total Lecture hours	æ	1	60 ho	urs		
Reference Boo		- CONTRACT RANK AND	1 and the					
		atics By Dr. P. Shanmughavel and C	Bulshan W	adhw	va, 20	010		
	laipur, India.	Usha & Dr.C.Jayaprakash						

Course Designed By: Dr.S.Usha & Dr.C.Jayaprakash

Mapping with Programme Outcomes COs **PO1 PO2 PO3 PO4 PO5 PO6 PO7 PO8 PO9 PO10** CO1 S S S S S S S Μ S S CO2 S Μ S Μ S S Μ S Μ S CO3 Μ S S Μ S S S S Μ Μ S S S S S S S **CO4** S S S